

VU Research Portal

Analysis of complex samples using multidimensional gas chromatography and selective detection

Stee, L.L.P.

2017

document version

Publisher's PDF, also known as Version of record

[Link to publication in VU Research Portal](#)

citation for published version (APA)

Stee, L. L. P. (2017). *Analysis of complex samples using multidimensional gas chromatography and selective detection*. [PhD-Thesis - Research and graduation internal, Vrije Universiteit Amsterdam].

General rights

Copyright and moral rights for the publications made accessible in the public portal are retained by the authors and/or other copyright owners and it is a condition of accessing publications that users recognise and abide by the legal requirements associated with these rights.

- Users may download and print one copy of any publication from the public portal for the purpose of private study or research.
- You may not further distribute the material or use it for any profit-making activity or commercial gain
- You may freely distribute the URL identifying the publication in the public portal ?

Take down policy

If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.

E-mail address:

vuresearchportal.ub@vu.nl

Contents

List of abbreviations.....	11
1 Introduction.....	13
1.1 General introduction.....	13
1.2 Scope of the thesis.....	15
2 Gas chromatography with atomic emission detection: a powerful and versatile technique.....	19
2.1 Introduction.....	19
2.2 Applications.....	21
2.3 Conclusions.....	39
3 Identification of non-target compounds using gas chromatography with simultaneous atomic emission and mass spectrometric detection (GC–AED/MS): analysis of municipal wastewater	41
3.1 Introduction.....	41
3.2 Experimental.....	42
3.3 Results and discussion.....	44
3.4 Conclusions.....	52
4 Comprehensive two-dimensional gas chromatography with atomic emission detection (GC×GC–AED) and correlation with mass spectrometric detection: principles and application in petrochemical analysis	53
4.1 Introduction.....	53
4.2 Experimental.....	54
4.3 Results and discussion.....	56
4.4 Application: petrochemical analysis.....	60
4.5 Conclusions.....	65
5 Evaluation of the combined use of biomimetic and solid-phase extraction techniques for the screening of organic micropollutants in wastewater.....	67
5.1 Introduction.....	67
5.2 Materials and methods.....	70

5.3	Results and discussion	73
6	Toxicity identification and evaluation of inland waters: Use of semi-permeable membrane devices and solid-phase extraction for the wide-range screening of microcontaminants in surface water by GC–AED/MS	83
6.1	Introduction	83
6.2	Experimental.....	84
6.3	Results	88
6.4	Conclusions	97
7	Responses in sediment bioassays used in the Netherlands: can observed toxicity be explained by routinely monitored priority pollutants?	103
7.1	Introduction	103
7.2	Materials and methods.....	104
7.3	Results	107
7.4	Discussion	109
7.5	Conclusions	111
8	Comprehensive two-dimensional gas chromatography (GC×GC) measurements of volatile organic compounds in the atmosphere.....	113
8.1	Introduction	113
8.2	Experimental.....	115
8.3	Results and discussion.....	119
8.4	Conclusions	130
9	Peak detection methods for GC×GC: an overview	137
9.1	Introduction	137
9.2	GC×GC: principles and visualisation	138
9.3	Classification of peak detection methods	140
9.4	Methods based on 1D peak detection	141
9.5	Multivariate techniques	153
9.6	Graphical drain method	159
9.7	Conclusions	161

10	Peak clustering in GC×GC–MS based on theoretical calculation of two-dimensional peak shapes: the 2DAid approach	165
10.1	Introduction	165
10.2	Theory	166
10.3	Experimental.....	170
10.4	Results and discussion	172
10.5	Conclusions	178
11	GC×GC–ToF-MS using various sets of column combinations for the non-target screening of 150 micro-contaminants detected in surface water.....	179
11.1	Introduction	179
11.2	Experimental.....	180
11.3	Results and discussion	181
11.4	Conclusions	185
12	References.....	187
	Samenvatting	199
	List of publications	203
	Dankwoord.....	205